

2-amino-3-(4-chlorophenyl)sulfonylpropanoic acid  
5445-04-5 | DTXSID30396827

Model Performance

Model	Data
-------	------

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

## Model Results

**Predicted value:** 307 °C

**Global applicability domain:** Outside

**Local applicability domain index:** 2.24e-01

**Confidence level:** 4.98e-01

## Nearest Neighbors from the Training Set

[Image not found](#)

Chloramben

**Measured:** 312

**Predicted:** 301

[Image not found](#)

Trimellitic anhydride

**Measured:** 390

**Predicted:** 366

[Image not found](#)

Benzoic acid, 2-benzoyl-

**Measured:** 261

**Predicted:** 309

[Image not found](#)

Ethyl oxanilate

**Measured:** 280

**Predicted:** 295